

Phase diagram of 2D array of mesoscopic granules.

A.I. Belousov, S.A. Verzhakov and Yu.E. Lozovik¹
Institute of Spectroscopy, Russian Academy of Sciences,
142092, Troitsk, Moscow region, Russia

A lattice boson model is used to study ordering phenomena in regular 2D array of superconductive mesoscopic granules, Josephson junctions or pores filled with a superfluid helium. Phase diagram of the system, when quantum fluctuations of both the phase and local superfluid density are essential, is analyzed both analytically and by quantum Monte Carlo technique. For the system of strongly interacting bosons it is found that as the boson density n_0 is increased the boundary of ordered superconducting state shifts to *lower temperatures* and at $n_0 > 8$ approaches its limiting position corresponding to negligible relative fluctuations of moduli of the order parameter (as in an array of "macroscopic" granules). In the region of weak quantum fluctuations of phases mesoscopic phenomena manifest themselves up to $n_0 \sim 10$. The mean field theory and functional integral $1/n_0$ - expansion results are shown to agree with that of quantum Monte Carlo calculations of the boson Hubbard model and its quasiclassical limit, the quantum XY model.

I. INTRODUCTION

The study of mesoscopic systems has resulted thus far in many new interesting fundamental concepts [2,3]. Progress has been especially rapid due to the development of nanotechnology methods which has opened up new avenues for sophisticated experiments. In this connection the study of arrays of ultrasmall granules, microclusters or Josephson junctions is of particular concern (see e.g. [4,5]).

Granular superconductors, Josephson arrays, superfluid helium in a porous media [6] are, as a rule, described in terms of different modifications of quantum XY model (see below), but this description is correct only if relative fluctuations of the local superfluid density are not essential [7]. It takes place in sufficiently large granules at temperatures far below that of onset of superconductivity in each individual granule. To study the role of quantum fluctuations of moduli other more adequate models should be used.

A convenient starting point for the description of the $N \times N$ system of interacting bosons (Cooper pairs in granules, He atoms in pores etc.) is the Bose - Hubbard Hamiltonian:

$$\hat{H}_h = \frac{t}{2} \sum_{\langle i,j \rangle} \{2a_i^\dagger a_i - a_i^\dagger a_j - a_j^\dagger a_i\} + \frac{U}{2} \sum_i \{a_i^\dagger a_i - n_0\}^2 \quad (1)$$

where a_i^\dagger (a_i) is a boson creation (annihilation) operator at a site $i = \overline{1, N^2}$; t is the strength of the hopping between nearest neighbor sites $\langle i, j \rangle$ and $U > 0$ is an on - site repulsive interaction.

The system (1) has a rich phase diagram [8,9], containing a Mott insulating phase (at zero temperature), the superfluid and normal (metal) phases. At a commensurate density $n_0 = \langle a_i^\dagger a_i \rangle$ (number of bosons is an integer multiple of the number of sites) and $T = 0$ the boson Hubbard model lies in the same universality class (see [8] - [10]) as the quantum XY model with Hamiltonian:

$$\hat{H}_{xy} = J \sum_{\langle i,j \rangle} \{1 - \cos(\varphi_i - \varphi_j)\} - \frac{U}{2} \sum_i \{\partial/\partial\varphi_i\}^2 \quad (2)$$

where $\varphi_i \in [0, 2\pi)$ are phases of the order parameter. Obviously, at $T \neq 0$ the requirements the density to be commensurate $n_0 = k$ is too stringent. In the latter case, the behaviour of the system (1) will depends *continuously* on n_0 , and the *critical* properties will be *the same* in some band $n_0 = k \pm \delta n_0$, the width $2\delta n_0$ should decrease as the temperature is lowered.

The properties of the system (2), that have at finite temperatures the superfluid and metallic phases are described by two dimensionless parameters: the temperature in units of Josephson coupling constant $T = k_b T/J$ and quantum parameter $q = \sqrt{U/J}$ which is responsible for the strength of zero - point fluctuations of phase. Corresponding parameters of the Hubbard model are $T = k_b T/(tn_0)$ and $q = \sqrt{U/(tn_0)}$.

The general purpose of this communication is comparing of phase diagrams of models (1) and (2) to estimate the importance of the mesoscopic phenomena in regular 2D systems. Of prime interest to us is the case of *finite temperatures*, apart of intriguing quantum phase transitions which take place at $T = 0$ (see e.g [11] and references therein). Sections II and III present the mean field and functional integral $1/n_0$ - expansion approaches. From *ab*

initio quantum Monte Carlo calculations of different characteristic quantities (Section IV) we determine the phase diagram $T_h^c(q; n_0)$ of the boson Hubbard model at different densities n_0 and compare it (Section V) with the phase diagram of 2D quantum XY model.

II. MEAN FIELD APPROXIMATION.

A qualitative estimation of the phase diagram of the boson model (1) can be obtained in a simple mean field approximation (see e.g. [12], [13,14] and references therein). The boundary $T^c(q; n_0)$ of ordered state can be found in MFA from the equation:

$$\frac{q^2}{z} = \frac{\sum_{n=-n_0}^{\infty} \{n + n_0 + 1\} \left\{ e^{-q^2[n-\eta]^2/[2T]} - e^{-q^2[n+1-\eta]^2/[2T]} \right\} / \{2n + 1 - 2\eta\}}{n_0 \sum_{n=-n_0}^{\infty} e^{-q^2\{n-\eta\}^2/[2T]}} \quad (3)$$

where $\eta = \mu/U - z/(2q^2n_0)$, z is the number of nearest neighbours ($z = 4$ for 2D square lattice). The Equation (3) on the boundary of ordered state differs in some details of that of the Reference [13]. Both of them became equivalent in the limit of large densities n_0 , with the Equation (3) more accurate at $n_0 \sim 1$.

The condition on the chemical potential μ is that the mean number of particles be equal to n_0 :

$$\sum_{n=-n_0}^{\infty} n \exp(-q^2\{n-\eta\}^2/[2T]) = 0 \quad (4)$$

It should be pointed out, that in the limit $n_0 \rightarrow \infty$ Equation (4) gives $\mu = 0$ and the boundary of ordered state transforms to that of quantum XY model [12].

The lines $T_h^c(q; n_0)$ of the boson Hubbard model obtained from Equations (3) and (4) are shown in Figure 1 for different densities n_0 . Calculation shows that the lines $T_h^c(q; n_0)$ reaches their limiting position, the phase boundary $T_{xy}^c(q)$ of quantum XY model at $n_0 > 25$.

III. $1/N_0$ - EXPANSION.

To improve the qualitative mean field estimation of the difference of phase diagrams of models (1) and (2) let us represent the partition function of the Hamiltonian (1) in a path integral representation as a trace over a complex c-number Bose field Φ [10]:

$$Z_h = \text{tr} \{ e^{-S} \} = \int D(\Phi, \Phi^*) e^{-S(\Phi, \Phi^*)}, \quad (5)$$

$$S(\Phi, \Phi^*) = \int_0^\beta \left\{ 1 \sum_i \dot{\Phi}_i \Phi_i^* + \frac{t}{2} \sum_{\langle i,j \rangle} |\Phi_i - \Phi_j|^2 + \frac{U}{2} \sum_i [|\Phi_i|^2 - n_0]^2 \right\} d\tau,$$

$$\Phi_i(0) = \Phi_i(\beta), \quad \Phi_i^*(0) = \Phi_i^*(\beta)$$

The substitution $\Phi_i = \sqrt{n_0 + \delta n_i} e^{i\varphi_i}$ (at integer n_0) in Equation (5) gives:

$$Z_h = \int D(\delta n, \varphi) e^{-S(\delta n, \varphi)}, \quad (6)$$

$$S(\delta n, \varphi) = \int_0^\beta \left\{ \frac{U}{2} \sum_i [\delta n_i]^2 + 1 \sum_i \delta n_i \dot{\varphi}_i \right.$$

$$\left. + t n_0 \sum_{\langle i,j \rangle} \left[1 + \frac{\delta n_i + \delta n_j}{2n_0} - \sqrt{(1 + \delta n_i/n_0)(1 + \delta n_j/n_0)} \cos(\varphi_i - \varphi_j) \right] \right\} d\tau,$$

$$\delta n_i \equiv n_i - n_0 = \delta n_i(\tau), \quad \varphi_i = \varphi_i(\tau).$$

From Equation (6) one can see, that increasing of the mean number of particles at each granule provided that $J = tn_0$ and U are constant, enables one to leave an action in terms of the phase degrees of freedom alone [7,10] to lead to the action of quantum XY model.

Being interested in the difference between phase boundaries of models (1) and (2) at sufficiently high but finite n_0 , let us expand the superfluid density in powers of $1/n_0$ up to a second order. Defining the superfluid density from the response of a system to the shift of phases at the boundary [15], from Equation (6) we have:

$$\nu_s = \gamma + \frac{1}{2n_0^2}\Gamma^{(2)} + \dots \quad (7)$$

where γ is the helicity modulus of quantum XY model [16,17]. The first order corrections are equal to zero due to the invariance of the action of the XY model against the "time" inversion.

Rather a complex expression for $\Gamma^{(2)}$ can be represented as some equilibrium value of quantum XY model [14], which can be easily estimated *via*. quantum Monte Carlo technique or different self-consistent approximations [18].

Given a value of the coefficient $\Gamma^{(2)}$ of the expansion (7) as a function of control parameters $\Gamma^{(2)} = \Gamma^{(2)}(q, T)$, one can construct an upper estimation of the phase boundary $T_h^c(q; n_0)$ of the boson Hubbard model (1):

$$T_h^c(q; n_0) \leq T_{xy}^c(q) \left\{ 1 + \frac{\nu_s(q, T_{xy}^c) - \gamma(q, T_{xy}^c)}{\gamma(q, T_{xy}^c)} \right\} = T_{xy}^c(q) \left\{ 1 + \frac{\pi\Gamma^{(2)}(q, T_{xy}^c)}{4n_0^2 T_{xy}^c(q)} \right\} \quad (8)$$

where $T_{xy}^c(q)$ is the line of topological phase transitions of quantum XY model (2). The estimation (8) can be easily obtained from the assumption that lines of phase transitions of both models are defined by the universal relation [16]:

$$\gamma(q, T_{xy}^c) = 2T_{xy}^c/\pi, \quad \nu_s(q, T_h^c) = 2T_h^c/\pi$$

Results of above mentioned estimations are given in Figure 1. It turns out that in the region $0.7 < q < 1.5$ the line of phase transitions of the Hubbard model approaches (to within 5%) its limit at $n_0 = 8$, whereas some greater densities $n_0 > 16$ are required in the strong quantum region $q > 1.7$ because of the rapid increase of the coefficient $\Gamma^{(2)}(q)$. Direct Monte Carlo calculation of the phase diagram $T_h^c(q)$ (see below), being in agreement with the predictions of $1/n_0$ - expansion at $0.7 < q < 1.5$, shows that in the case of *strongly* interacting system (at $q > 1.7$) theoretical estimations markedly overestimate the maximum boson density n_0 at which mesoscopic effects are still essential.

To conclude of this chapter one additional feature should be recognized. It is easy to see, that all estimations presented in this Section and started from the partition function (5) have been carried out in the *grand canonical* ensemble with zero chemical potential. This has enabled us to make all calculations analytically, disregarding the restrictions on the total number of particles in the system when integrating over the fluctuations of moduli of the order parameter. In order to justify the possibility of comparing the MC results with theoretical estimations it is need to show that, being calculated within the same approach, the discrepancy δn between the mean number of bosons per granule and n_0 is small.

From (6) for δn one can write

$$\delta n = \frac{1}{n_0}\Delta^{(1)} + \dots \quad (9)$$

As calculation shows, the value of $\Delta^{(1)}$ is less than 0.1 in the region $q > 0.7$, $T < 1$. This observation justifies our use of great canonical ensemble with zero chemical potential in estimating the coefficient $\Gamma^{(2)}$ of series (7).

IV. QUANTUM MONTE CARLO SIMULATIONS.

In studies of properties of the boson Hubbard model (1) at different values of control parameters $\{q, T\}$ we have applied the "checkerboard" breakup [19]. In this method the classical degrees of freedom to be sampled are imaginary - timedependent boson occupation number field $\{n_i^p\}$, $i = 1 \dots N^2$, $p = 0 \dots 4P$. The algorithm of Monte Carlo (MC) calculations of the quantum XY model was described in [17,20]. We have performed extensive tests to verify that our results converge in the limit of $P \rightarrow \infty$. Results presented below have been obtained by the averaging over 3 - 5 initial configurations formed by $4P$ - times (P - times for the XY model) multiplication of the random configuration of bosons (phases for the XY model) at the lattice $N \times N$.

The main attention has been given to the calculation of the superfluid density ν_s . This quantity have been determined from the winding number [9,19]

$$\nu_s = 0.5T \langle W_{\mathbf{x}}^2 + W_{\mathbf{y}}^2 \rangle_{\mathbf{h}} \quad (10)$$

$$W_{\mathbf{x}} = \sum_{p=0}^{4P} \sum_{i_y=1}^N (-1)^{i_x+p} n_i^p, \quad W_{\mathbf{y}} = \sum_{p=0}^{4P} \sum_{i_x=1}^N (-1)^{i_y+p} n_i^p,$$

where n_i^p means the number of bosons at a site i (with coordinates $\{i_x, i_y\}$) of a level p of 3D classical system. We have also used the current autocorrelation function [21]

$$\nu_s = -\frac{1}{n_0 N^2} \langle \hat{T}_{\mathbf{x}} \rangle_{\mathbf{h}} - \frac{1}{n_0^2 N^2 T P} \sum_{\tau=0}^{P-1} \langle \hat{J}_{\mathbf{x}}^{(p)}(\tau) \cdot \hat{J}_{\mathbf{x}}^{(p)}(0) \rangle_{\mathbf{h}} \quad (11)$$

$$\hat{T}_{\mathbf{x}} = -\frac{1}{2} \sum_i \{a_{i+x}^\dagger a_i + a_i^\dagger a_{i+x}\},$$

$$\hat{J}_{\mathbf{x}}^{(p)} = -\frac{\hat{J}}{2} \sum_i \{a_{i+x}^\dagger a_i - a_i^\dagger a_{i+x}\}, \quad \hat{J}_{\mathbf{x}}^{(p)}(\tau) = e^{\tau \beta \hat{H}/P} \hat{J}_{\mathbf{x}}^{(p)} e^{-\tau \beta \hat{H}/P}$$

The substitution $a_i \rightarrow \sqrt{n_0} e^{i\varphi_i}$ transforms Equation (11) to the well - known expression for the helicity modulus γ of the quantum XY model [17].

As have been pointed out by Scalapino et. al. [22], the temperature derivative of the superfluid density gives an additional information about the type of phase transition at some temperature $T^c(q)$: in framework of the Kosterlitz - Thouless picture the value of $\partial(\beta\nu_s)/\partial\beta$ scales to a Dirac delta function $\delta(T - T^c)$. On the finite lattices $\partial(\beta\nu_s)/\partial\beta$ shows a response which increases with lattice size N , the position of the maximum of the derivative being independent on N .

To find the derivative of the superfluid density $\partial(\beta\nu_s)/\partial\beta$ we have estimated the difference in internal energies of systems which differ by a phase twist $\delta\varphi$ in the boundary condition along one lattice direction.

$$\frac{\beta\{E(\delta\varphi) - E(0)\}}{n_0 \beta t} \sim \nu_s + \beta \frac{\partial \nu_s}{\partial \beta} \quad (12)$$

One can show, that for the Cooper pairs of charge $2e$ this phase twist can be realized in the "flux quantization" scheme and is equivalent to threading a flux through the center of a torus on which the system lies [22].

We have also calculated the fluctuation of bosons at lattice sites

$$\delta n_{\mathbf{h}}^2 = \frac{1}{4PN^2} \left\langle \sum_{p=0}^{4P-1} \sum_i \{n_i^p - n_0\}^2 \right\rangle_{\mathbf{h}} \quad (13)$$

V. RESULTS AND DISCUSSION.

Shown at Figure 2 are dependencies of the superfluid fraction $\nu_s(T)$ of the Hubbard model at $q = 0.2$ (in the classical region of XY model (2), Figure 2a) and $q = 2.0$ (see Figure 2b). For reference, the helicity modulus γ of quantum XY model as function of temperature T is also plotted. Analysis of data obtained at different sizes N and densities n_0 of the system reveals that for the system of strongly interacting bosons (at $q = 2.0$) the MC results are in qualitative agreement with the theoretical estimations of Sections II and III. Really, from Figures 1 and 2 one can see that as the density of bosons n_0 is increased, the boundary of ordered superconducting state of the system (1) approaches that of quantum XY model with critical temperatures $T_{\mathbf{h}}^c$ of the Hubbard model being greater than $T_{\mathbf{xy}}^c$ of quantum XY model. The line of transitions $T^c(q)$ can be estimated from the universal relation $\nu_s(T^c) = 2T^c/\pi$. Thus defined, the temperature of metal - superconductor transition agree fairly well with the position of the peak of the temperature derivative of superfluid density (12). Our calculation shows, that the position of the maximum of the derivative does not depend (to within statistical errors) on the system size and, as one can see from Figure 3, lowers as n_0 is increased.

From Figure 2a one can show, that the transition temperature of the weakly interacting bosons (at $q = 0.2$) appeared to be *less* than that of quantum XY model. This tendency persists with increasing the system size. The theoretical approach used in Section III can not help to elucidate the reason of this phenomena because at $q < 0.4$ relative fluctuations of moduli of the order parameter are only weakly damped by the interaction, corrections $\Gamma^{(2)}$ and $\Delta^{(1)}$ are large and theoretical estimations work badly.

Let us consider the behaviour of $\nu_s(q)$ and $\gamma(q)$ as functions of quantum parameter q at $T = 0.5$ (see Figure 4). Defining the point q^c of phase transition from the universal relation $\nu_s(q) = 2T/\pi$ we see that the boundary of ordered superconducting state of the model (1) lies to the right of the boundary of the model (2). This conclusion is verified by the results of calculations of the derivative $\partial(\beta\nu_s)/\partial\beta$ presented at the insert of Figure 4. The position $q|_{n_0=3} \approx 2.3$ of a peak of the derivative is in a sufficiently good agreement with the critical point $q^c|_{n_0=3} \approx 2.4$ determined from the universal relation.

The dependence of the relative fluctuation of particle number at sites of the system *vs.* quantum parameter q is shown at Figure 5. Particularly, Figure 5 can serve as an illustration of the role of interaction in the transition to the quasiclassical limit from the boson Hubbard to quantum XY model. Really, at finite densities n_0 the spectrum of the operator $\hat{n}_i - n_0$ can be considered as unbounded only if relative fluctuations of particle number are small $\delta n_{\mathbf{h}}^2/n_0^2 \ll 1$. Then, as it is usually done on examination Josephson or granular systems in terms of the model (2), the particle number operator $\hat{n}_i - n_0$ can be chosen as a conjugate one to the "phase" operator $\hat{\varphi}_i$: $\hat{n}_i - n_0 = i\partial/\partial\varphi_i$. Increasing of the interaction (quantum parameter q) leads to the suppressing of the relative fluctuations of the order parameter module as can be seen from Figure 5. It should be noted, that at high q the fluctuations of particles number are *greater* than those of quantum XY model and approach their with increase in density. The results presented in the insert of the Figure are relative fluctuations $\delta n_{\mathbf{h}}^2/n_0^2$ as functions of quantum parameter q at $T = 0.5$ at different densities n_0 . The increase in n_0 is seen to be of great importance in suppressing the relative fluctuations.

A great attention has been given thus far to the possibility of *reentrance* phenomena, when the global superconducting state in some region of q is absent not only at high, but also at sufficiently low temperatures. In the framework of XY model the possibility of this phenomenon taking place has been connected with the domain of phases [12], dissipation or mutual capacitances effects [23,24]. From results presented one can see that taking into account the fluctuation of moduli of the order parameter does not lead to the reentrance phenomena at least in the region explored.

To conclude, we have used the boson Hubbard model to analyze the effect of quantum fluctuations of phases and moduli of the order parameter on the onset of superconductivity in 2D mesoscopic Josephson system. Both mean field approximation and $1/n_0$ expansion leads to the conclusion that the line $T^c(q)$ of superconductor - metal phase transitions lies *above* that of quantum XY model, the latter being quasiclassical limit (as $n_0 \rightarrow \infty$, $U \neq 0$) of the Hubbard one. Our MC simulations show that in the region $q < 1$ of small quantum fluctuations of phases it needs an average of 10 bosons per site to suppress relative fluctuations of the local superfluid density. As interaction is increased, the quasiclassical limit is approached at lower densities ($n_0 \sim 8$ at $q \sim 2$). No reentrance or discontinuity phenomena have been found.

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Figure 1.

The phase diagram of 2D Hubbard (1) and quantum XY (2) models. S - superconducting, N - normal state. The mean - field results: **1**: $n_0 = 1$, **2**: $n_0 = 2$, **3**: $n_0 = 6$, **4**: quantum XY model ($n_0 = \infty$); The $1/n_0$ expansion (8) results: **5**: $n_0 = 6$, **6**: $n_0 = 14$. Symbols present points of phase transitions have been found by MC method.

Figure 2a.

The superfluid density ν_s (helicity modulus γ) *vs.* temperature T at $q = 0.2$. The dependence $2T/\pi$ (see in text) is given by a dashed line. Data are connected to guide the eyes. If not presented, error bars are within the size of the data point.

Figure 2b.

The superfluid density ν_s (helicity modulus γ) *vs.* temperature T at $q = 2.0$.

Figure 3.

$T\beta\{E(\pi/2) - E(0)\}/\{n_0 N^2\}$ as a function of temperature T . The solid lines are spline fits to the data.

Figure 4.

The superfluid density ν_s (helicity modulus γ) *vs.* quantum parameter q at $T = 0.5$. The line $1/\pi$ is shown with the help of a dashed line.

Insert: the temperature derivative of the superfluid fraction (12).

Figure 5.

Fluctuation $\delta n_{\mathbf{h}}^2$ of the number of bosons at sites of the system as a function of quantum parameter q at $T = 0.5$. Insert: relative fluctuations $\delta n_{\mathbf{h}}^2/n_0^2$ at different densities n_0 .











